

Chaotic temperature dependence in a model of spin glasses

A Random-Energy Random-Entropy model

F. Krzakala¹ and O.C. Martin^{1,2}

¹ Laboratoire de Physique Théorique et Modèles Statistiques, bât. 100, Université Paris-Sud, F-91405 Orsay, France

² Service de Physique de l'État Condensé, Orme des Merisiers — CEA Saclay, 91191 Gif sur Yvette Cedex, France.

February 1, 2008

Abstract. We address the problem of chaotic temperature dependence in disordered glassy systems at equilibrium by following states of a random-energy random-entropy model in temperature; of particular interest are the crossings of the free-energies of these states. We find that this model exhibits strong, weak or no temperature chaos depending on the value of an exponent. This allows us to write a general criterion for temperature chaos in disordered systems, predicting the presence of temperature chaos in the Sherrington-Kirkpatrick and Edwards-Anderson spin glass models, albeit when the number of spins is large enough. The absence of chaos for smaller systems may justify why it is difficult to observe chaos with current simulations. We also illustrate our findings by studying temperature chaos in the naïve mean field equations for the Edwards-Anderson spin glass.

PACS. 75.50.Lk Spin glasses and other random magnets – 05.70.Fh Phase transitions: general studies – 64.70.Pf Glass transitions

1 Introduction

It is generally agreed that the equilibrium states of spin glasses [1,2] are “fragile”, i.e., they are sensitive even to very small perturbations. Roughly, this can be argued from the fact that there exist many (meta-stable) states whose excess free-energies grow more slowly than the system’s volume; then arbitrarily small extensive perturbations will re-shuffle the different (meta-stable) states and the lowest free-energy state will be completely different from the one without the perturbation. This phenomenon is referred to as “chaos” [3] as the equilibrium state depends chaotically on the perturbation. In particular, there has long been a consensus that chaos arises when changing the couplings J_{ij} between the spins. However, the situation is quite different when the parameter being changed is the temperature; though earlier work [4,5] claimed that there is chaos under even infinitesimal temperature changes, some recent work goes against this; indeed, analytic expansions [6] around the critical temperature give no temperature chaos in the Sherrington-Kirkpatrick (SK) model, and extensive Monte Carlo simulations in both the three-dimensional Edwards-Anderson (EA) model and the SK model find little or no evidence of temperature chaos [7, 8].

This controversy is interesting in itself as it shows just how poorly understood spin glasses remain after years of work. More importantly perhaps, temperature chaos plays

a central role in many theoretical descriptions of dynamics. Indeed, phenomena such as rejuvenation [9] that follow temperature changes in glassy systems must arise if there is temperature chaos (see for instance [10] and [11]). Thus both for equilibrium and for non-equilibrium properties, it is appropriate to understand whether or not there is temperature chaos in disordered systems, and in spin glasses in particular.

In this work, we present a solvable glassy model where the temperature dependency is easily analyzed. Our main result is that the presence of temperature chaos depends on an exponent associated with state-to-state entropy fluctuations. Depending on the value of this exponent, the model exhibits strong, weak, or no chaos at all. When extrapolating these results to realistic models, we find chaos both for the SK and EA models but only when the number of spins N is quite large, $O(1000)$. This may justify why chaos is not seen in Monte-Carlo simulations. Finally, we attempt to confirm numerically these predictions by using a naïve mean field approximation; there we also find the expected signatures of a chaotic temperature dependence.

This paper is organized as follows. In section 2, we motivate and explain this study; our Random-Energy Random-Entropy Model is described and solved in section 3. In section 4, we determine how the equilibrium state changes with temperature. In section 5, we generalize this model to the droplet/scaling picture. In section 6, we discuss the predictions coming from another simple spin glass system

based on the naïve mean field equations. We summarize and conclude in section 7.

2 Temperature chaos as level crossings

Our framework is motivated by the concept of “valleys” in glassy systems. Indeed, within the mean field picture of disordered systems in their low temperature frozen phase, ergodicity is broken and configuration space is broken into many components not related by symmetry. These components are often referred to as valleys as in an energy landscape picture. Loosely, one considers each valley to be associated with one thermodynamic “state”, though such an association has ambiguities, especially in finite volume. This picture of valleys is *not* restricted to a mean field framework: even in the droplet [12] and scaling [13] pictures, the energy landscape is very rugged and there exist multiple valleys corresponding to possibly (meta-stable) states that do not contribute to equilibrium properties in the thermodynamic limit. We will thus assume that we can talk of states (equilibrium or meta-stable) and then ask within such a picture what can be said about temperature chaos.

2.1 Level crossings

In the simple case of the ferromagnetic Ising model below its critical temperature T_c , there are two valleys \mathcal{V}_1 and \mathcal{V}_2 with degenerate free-energies and magnetizations $\pm m(T)$. Consider the mean spin-spin overlap $q^{1,2}$ between these valleys: it is $q^{1,2} = -m^2(T)$. The associated (equilibrium) states have a smooth evolution with temperature, merging when T approaches T_c from below. It is also possible to consider the overlaps between an equilibrium state at T and one at $T + \delta T$. Such an overlap is equal to $\pm m(T)m(T + \delta T)$, which also varies smoothly with T and δT . On the contrary, to have temperature chaos, we want such overlaps to be very sensitive to δT , and generically one expects the equilibrium states at different temperatures to be “totally different”, meaning their overlap is zero (in the absence of an external field).

Does one have temperature chaos in disordered systems where the abundance of (meta-stable) states plays a fundamental role? The answer is yes for spin glasses on Migdal-Kadanoff hierarchical lattices [14,15] or for other disordered systems like the Directed Polymer in a Random Medium in 1+1 dimension [16,17]. But in other systems one might instead expect that a state dominating the partition function at T will also dominate it at $T + \delta T$. Such a scenario is represented pictorially on the left of figure 1 where for each state we plot its free-energy as a function of temperature. We can think of these curves as a family of levels, and in this case there are no level crossings. Interestingly, this is what occurs in the the infinite range *spherical* p-spin model [18]. There one can define states in the large volume limit, for instance by the Thouless-Anderson-Palmer (TAP) [19] equations. These different states evolve smoothly with temperature, and furthermore

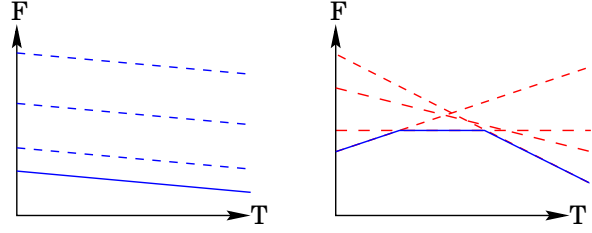


Fig. 1. Temperature dependence of free-energies of the lowest states. (a): there are no entropic fluctuations, as in the spherical p-spin model; (b) possible level crossing behavior in more realistic models.

have zero mutual overlap. When following analytically the free-energy of these states as a function of temperature, one finds that they keep the same order: there are *no level crossings*.

Although such a property may be special to the spherical p-spin model, there is also the possibility that it is more general, extending to all mean field models or even to finite dimensional models; this is supported by the lack of any numerical evidence in favor of chaos in either the SK model or the Edwards-Anderson model.

2.2 The Bray and Moore argument

To understand why many researchers expect a chaotic temperature dependence in finite dimensional spin glasses, it is of some use to go over the argument due to Bray and Moore (BM) [3], reformulated for our particular purposes. For specificity, we work with the 3-dimensional EA model with no magnetic field whose Hamiltonian is

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j \quad (1)$$

The S_i are Ising spins on an $L \times L \times L$ lattice and the sum is over nearest neighbor sites with periodic boundary conditions; the J_{ij} are independent Gaussian random variables. We start from two “states” at low temperature, differing by a very large droplet and work in the framework of the droplet/scaling theory of spin glasses [13,20]. The two states have free-energies that differ by $\Delta F(T) = \Delta E - T\Delta S \approx \Upsilon \ell^\theta$, where ℓ is the characteristic size of the flipped droplet when going from state 1 to state 2 and Υ is the temperature dependent stiffness coefficient. Now change the temperature; $\Delta F(T + \delta T) \approx \Delta E - (T + \delta T)\Delta S$, so that $\Delta F(T + \delta T) \approx \Upsilon \ell^\theta - \delta T \Delta S$.

Following Bray and Moore, it seems inevitable that the entropy difference is associated with the droplet’s surface so that ΔS has a random sign and a typical magnitude proportional to $\ell^{d_s/2}$ where d_s is the fractal dimension of the droplet’s surface. Then if $d_s/2 > \theta$, which follows from the inequality $\theta < (d-1)/2$, the difference in free-energies $\Delta F(T + \delta T) \propto \Upsilon \ell^\theta + \delta T \ell^{d_s/2}$ can change sign between T and $T + \delta T$. The conclusion is then that the equilibrium state(s) between T and $T + \delta T$ should change on a length

scale ℓ scaling as $\ell(\delta T) \propto \delta T^{-1/(\frac{d}{2}-\theta)}$ while their typical overlap $q_{T,T+\delta T}$ should go to zero as

$$q_{T,T+\delta T} \approx \left(\frac{\ell(\delta T)}{L} \right)^{d/2} \quad (2)$$

where L is the total lattice size. In the droplet/scaling picture, $\theta \approx 0.2$, while in the mean field picture $\theta = 0$; in either case, the argument strongly suggests that the EA model has temperature chaos. At the root of the argument are large cancellations between E and S in the equilibrium value of F ; these cancellations make the equilibrium state very sensitive to changes in T . Note that numerical evidence for such cancellations has been found [21] in the $3-d$ EA model. Finally, as mentioned previously, chaos does occur on the Migdal-Kadanoff lattice;

To us, the Bray and Moore argument is very convincing if one goes from $T = 0$ to $T = \epsilon$ for any $\epsilon > 0$, suggesting that chaos is unavoidable at $T = 0$. However, the argument has potential pitfalls when considering chaos at $T > 0$. First, when going from T to $T + \delta T$, both ΔE and ΔS change, a fact which is neglected in the argument. Second, one cannot treat a single scale ℓ alone; it is possible that the *droplets* on the scale smaller than ℓ will see their free-energy change sign, and thus the “evolution” of $\mathcal{V}_1(T)$ to $T + \delta T$ will differ from $\mathcal{V}_1(T)$ by many droplet excitations. This evolution may be enough to keep the free-energy of $\mathcal{V}_1(T + \delta T)$ below that of $\mathcal{V}_2(T + \delta T)$. In this sense, the chaos at scale $\ell(\delta T)$ might be quenched by the way the equilibrium state *adapts* to changes in T . And since $\mathcal{V}_1(T)$ and $\mathcal{V}_1(T + \delta T)$ differ only by droplet excitations, their overlap will not be close to zero. Unfortunately we cannot take into account these effects in a realistic way; nevertheless, we want to use the fact that the state dominating the partition function at one temperature is quite special, being the result of an extreme statistic where the free-energy is optimized for that temperature. We now proceed to see how we can model this.

3 The Random-Energy Random-Entropy Model

In the Bray and Moore argument, the important feature is that there are very large entropy fluctuations from state to state. We shall now define a glass model that incorporates such entropy fluctuations. Since our model is close to Derrida’s Random Energy Model [22](REM), we have named it the *Random-energy Random-entropy model* (Re-Rem). In the spirit of the REM, we start by taking 2^N “valleys”, each with an energy taken from a Gaussian distribution, but we shall also assign a random entropy to each valley.

3.1 Definition of the Re-Rem

The Re-Rem model is defined as follows. We have 2^N states; the *free-energy* of state i is given by

$$F_i = E_i - TS_i \quad (3)$$

where E_i and S_i are random independent variables, taken from a Gaussian distribution of mean 0 and standard deviation $\sigma_E = N^{0.5}/\sqrt{2}$ for the energy and $\sigma_S = N^\alpha/\sqrt{2}$ for the entropy, α being an exponent that will play an essential role later. More explicitly, these probability distributions are

$$\rho_E(E_i) = \frac{\exp\left(-\frac{E_i^2}{N}\right)}{\sqrt{N\pi}} \quad \rho_S(S_i) = \frac{\exp\left(-\frac{S_i^2}{N^{2\alpha}}\right)}{\sqrt{N^{2\alpha}\pi}} \quad (4)$$

Note that for the E_i , the probability distribution is the same as in the REM. A simple way to visualize this model is to think to 2^N lines in a temperature-free-energy plot as in figure 1 where the intercept on the y axis is random as well as the slope of each line.

Being the sum of independent Gaussian random variables, the free-energy has a Gaussian distribution. Thus F has zero mean and variance $\sigma_F^2 = \sigma_E^2 + \sigma_S^2$. Explicitly, the variance of the free-energies satisfies

$$2\sigma_F^2 = N + T^2 N^{2\alpha} \quad (5)$$

If $\alpha = 1/2$, the two terms contribute the same magnitude at large N , while if $\alpha < 1/2$, the variance is dominated by σ_E . The natural scaling then seems to be $\alpha = 1/2$ in which case the ground state energies and entropies are both extensive. In a T-F plot, we may expect these states to have crossings, like in the right part of figure 1.

3.2 The equivalent REM

Because of the Gaussian distribution of free-energies at each temperature T , the model is equivalent to a REM whose energy variance is given by equation 5. This allows one to solve the thermodynamics of the model. The density of levels with free energy F is

$$\rho_F(F) = 2^N \frac{e^{-\frac{F^2}{2\sigma_F^2}}}{\sigma_F \sqrt{2\pi}} \quad (6)$$

As expected, there is a critical dependence on F for large N . If $|F| < F_0 = \sigma_F \sqrt{2N \ln 2}$, there is an exponentially large density of states and an extensive *configurational* entropy

$$S_C(F) = N \ln 2 - \frac{F^2}{2\sigma_F^2} \quad (7)$$

whereas if $|F| > F_0$, there are no levels at all in the thermodynamic limit and thus $S_C(F) = 0$. Using the relation between configurational entropy and temperature $T^{-1} = \partial S_C / \partial F$, the critical temperature is

$$T_c = \frac{\sigma_F}{\sqrt{2N \ln 2}} \quad (8)$$

and thus T_c satisfies the self-consistent equation

$$T_c = \frac{\sqrt{N + T_c^2 N^{2\alpha}}}{2\sqrt{N \ln 2}} = \sqrt{\frac{1 + T_c^2 N^{2\alpha-1}}{4 \ln 2}} \quad (9)$$

This lead us to distinguish three cases. First, if $\alpha < 0.5$, then $T_c = 1/(2\sqrt{\ln 2})$, as in the original REM. There is a low temperature phase in which the partition function is dominated by a finite number of states (those with the lowest free-energies); the entropy density in this phase is zero. There is also a high temperature phase for which the number of states that contribute to the partition function is exponentially large in N . Second, for $\alpha = 0.5$, one finds that $T_c = \frac{1}{\sqrt{4\ln 2 - 1}} \approx 0.75$. The physics is the same as before, but the critical temperature is shifted. In both cases, we have a glassy model with a one-step replica symmetry breaking transition [22,23]. Third, if $\alpha > 0.5$ one finds $T_c = +\infty$; there is no phase transition, and the systems remains in the “low temperature phase” at all temperatures. This can be considered to be unphysical because a microscopic Hamiltonian such as Eq 1 will always have a high temperature disordered phase. If we go back to the Bray and Moore argument, in which entropy fluctuations grows as $l^{d_s/2}$, we see that we should identify the Re-Rem parameter α with $d_s/(2d)$. Happily, if one follows the prescription $\alpha = d_s/(2d)$, there is no unphysical behavior because $d_s \leq d$, so $\alpha \leq 0.5$.

Note that when $\alpha \leq 0.5$, the lowest free-energies scale linearly with N and the gap between the lowest free-energy state and the first excitation is $O(1)$, as in the REM. Furthermore if $\alpha < 0.5$, the lowest free-energy density does not change with T , whereas if $\alpha = 0.5$, it grows as $\sqrt{1+T^2}$. Finally in the case $\alpha > 0.5$, the free-energy grows as $N^{\alpha+0.5}$ and thus is not extensive.

3.3 Energy and entropy

The lowest free-energy in the Re-Rem at each temperature is easily found, and from it we can determine the typical energy and entropy at each temperature. The lowest free-energy at each temperature is given by [22]

$$F_0 \approx -\sqrt{2N \log 2} \sigma_f = -N \sqrt{\log 2 (1 + T^2 N^{2\alpha-1})} \quad (10)$$

The entropy in the low T phase is obtained from the derivative of this free-energy with respect to temperature:

$$S_0 \approx \frac{\sqrt{\log 2} T N^{2\alpha}}{\sqrt{1 + T^2 N^{2\alpha-1}}} \quad (11)$$

which confirms that the entropy is extensive only for $\alpha = 0.5$. To determine the energy we use,

$$E_0 = F_0 + T S_0 \approx -\frac{N \sqrt{\log 2}}{\sqrt{1 + T^2 N^{2\alpha-1}}} \quad (12)$$

The energy is thus extensive if $\alpha \leq 0.5$.

4 Level crossings in the Re-Rem

Given our model with many states and a spin glass phase, we focus on the problem of level crossings. We have 2^N

levels and randomness in entropy and energy. We want to follow the lowest free-energy state and see if this state changes with temperature, and how often it does if so. First, we will provide some analytical constraints, deriving a scaling law governing the number of crossings in a δT interval; then we will determine the corresponding scaling function by a numerical computation.

4.1 Level crossings via thermodynamics

At $T = 0$, the lowest level is the one with the minimum energy, entropy plays no role. If one follows the line starting from this minimum energy in temperature, we can expect some other levels, with larger energies but also more negative entropies, to cross this line. This is what happened in the Bray and Moore analysis, showing that zero temperature chaos is inevitable. But what happens at $T > 0$? Does the lowest free-energy state change at each temperature? What is the density of crossings? The problem of knowing which level is lowest at each temperature and of computing crossing statistics seems rather non-trivial; however thanks to the mapping to the REM, it is possible to compute the temperature dependence of the best level, and to deduce from that many properties of the crossings.

Let us begin with some remarks. First, the role of the exponent α is just to rescale the temperature definition by a factor N^α as is evident from equation 3. Thus if one solves the problem for $\alpha = 0$, changing to an $\alpha \neq 0$ just divides each crossing temperature by N^α . As a consequence, the total number of crossings does not depend on α . Second, this total number of crossings (the number of times the lowest free-energy level changes its slope) is at most of $O(N)$. This can be shown using the following argument. Take all 2^N states and consider the lowest one \mathcal{L}_1 at $T = 0$. The entropy is random and uncorrelated with the energy, so if you take the next state \mathcal{L}_2 in energy, you will have a good chance (50%) that it will have a more negative entropy and thus will cross \mathcal{L}_1 . Suppose this is the case. A further state \mathcal{L}_i with a still greater energy will cross \mathcal{L}_2 only if its slope is more negative than that of \mathcal{L}_2 . The entropy of a successful candidate \mathcal{L}_i must be the lowest of i entropies taken at random. Since by hypothesis \mathcal{L}_2 has the lowest entropy of 2 entropies taken at random, we have to let i go up to 4 to have a 50% chance of finding a state that will cross \mathcal{L}_2 . Extending this argument, to get the k^{th} crossing one will need to examine $O(2^k)$ successive levels. Furthermore, it is not difficult to show that when going from \mathcal{L}_{2^k} to $\mathcal{L}_{2^{k+1}}$ the energy increases by $O(1)$.

Of course, these $O(N)$ crossings are not the end of the story because some of them may be irrelevant. Take for example the right part of figure 1 where the third energy state crosses the second one, but where the fourth one crosses the second one *before* the third does. From this simple example we see that not all crossings count; we can only say that the number of levels that become at some point the state of lowest free-energy is at *most* $O(N)$, and that the energy at each level crossing increases by at *least* $O(1)$.

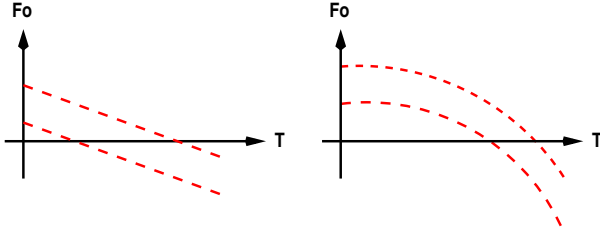


Fig. 2. The lowest states in the Re-Rem remain inside a “tube”. Left: $\alpha > 0.5$, the dependence is linear in T ; right: $\alpha \leq 0.5$ the tube is curved.

In the large N limit, a scaling behavior sets in. But before being quantitative, let us see what qualitative properties imply level crossings. The starting point is the fact that, at fixed T , the Re-Rem reduces to a REM. The lowest free-energy at each temperature scales as in equation 10 and its sample to sample fluctuations are of $O(1)$. Thus the lowest state resides in a “tube” (see figure 2) in the (T, F) diagram. Clearly, if the tube is not linear in temperature, there must be some level crossings. We will now see how this imposes strong constraints on the crossing statistics.

First, consider the case where $\alpha > 0.5$. At large N , we get

$$F_0 \propto -N^{\alpha+0.5}T \quad (13)$$

The linear temperature dependence suggests that the tube has one, or just of few states passing through it for all T . Moreover the slope of this tube is of $O(N^{\alpha+0.5})$ which is the scale for the lowest entropy value obtained by taking 2^N values in a Gaussian of variance $N^{2\alpha}$. So if at $T = 0$, the best state is the one with lowest E , at any strictly positive temperature the best state is the one with the best slope. This means that all level crossings take place at zero temperature; there is zero temperature chaos but no chaos at $T > 0$!

When $\alpha \leq 0.5$, we have

$$F_0 \approx -N\sqrt{\ln 2} - \frac{N^{2\alpha}\sqrt{\ln 2}T^2}{2} \quad (14)$$

Now, the dependence in T is non-linear; there must be some crossings at $T > 0$ because the lowest energy state changes its slope in temperature and in N . This suggests that the number of crossings in a δT interval diverges with N for every temperature.

Finally, if $\alpha = 0$, we obtain

$$F_0 \approx -N\sqrt{\ln 2} - \sqrt{\ln 2}T^2 \quad (15)$$

so the dependence on T is N -independent. Since the energy increase of successive crossings is at least of $O(1)$, it is not possible to pass an infinite number of levels in the tube. Thus there should only be a finite number of crossings in each δT interval.

Now we also know that changing α is the same as re-scaling the temperature; this gives a strong constraint on the number of crossings in a given interval. Let's assume

that the scaling of the mean number of crossings in a temperature interval δT is of the form

$$\mathcal{N}_N(T, T + \delta T) = N^{\gamma(\alpha)}\delta T g\left(\frac{T}{N^{\kappa(\alpha)}}\right) \quad (16)$$

Then the invariance under the transformation $\alpha_1 \rightarrow \alpha_2$ and $T \rightarrow TN^{\alpha_1 - \alpha_2}$ gives

$$\begin{aligned} \gamma(\alpha_1) - \gamma(\alpha_2) &= \alpha_1 - \alpha_2 \\ \kappa(\alpha_1) - \kappa(\alpha_2) &= \alpha_2 - \alpha_1 \end{aligned} \quad (17)$$

It follows that

$$\begin{aligned} \gamma(\alpha) &= \alpha + \beta_1 \\ \kappa(\alpha) &= -\alpha + \beta_2 \end{aligned} \quad (18)$$

Furthermore, we must respect the constraints derived previously. First, assuming $g(x)$ decays quickly (not as a power law) at large x , the disappearance of $T > 0$ crossings when $\alpha > 0.5$ gives $\beta_2 = 0.5$. Second, since $\alpha = 0$ gives crossing density at large N , we must have $\beta_1 = 0$. The scaling form for the mean number of crossings in a temperature interval δT is then

$$\mathcal{N}_N(T, T + \delta T) = N^\alpha \delta T g\left(\frac{T}{N^{0.5-\alpha}}\right) \quad (19)$$

From this formula, we deduce that the total number of crossings is in fact $O(\sqrt{N})$, much less than the bound $O(N)$. Also if $g(0)$ is finite, the case $\alpha = 0$ leads to a mean temperature of the k^{th} crossing that is proportional to k .

4.2 Numerical investigation

It is of some use to illustrate and check these results by a numerical procedure but we also want to compute the function $g(x)$. A simple way to do this is to generate 2^N random energies, 2^N random entropies, and to check for crossings, but such a procedure requires a computation time that is exponential in N . Instead we used a method which allows us to have an algorithm linear in N , and thus to simulate up to 2^{800} levels. With no loss of generality we can focus on the case $\alpha = 0$; we have simulated 10000 instances for $N = 100, 200, 300, 400, 600$ and 800 .

We explain our algorithm in the appendix for readers interested in algorithmic issues. Basically, our method constructs in a time proportional to N the series of crossing points for a random realization of the Re-Rem. Then we measure the statistics of these crossings by averaging over many instances, repeating this for different values of N . The scaling function $g(x)$ is then obtained by using equation 19; the results are shown in figure 3. The data collapse is excellent, showing that the T/\sqrt{N} scaling works very well. We do see some deviations at small N in the tail; these correspond to corrections to scaling, and are small (invisible) beyond $N = 500$.

From this numerical computation of $g(x)$, we can extract the number of crossings in any temperature interval

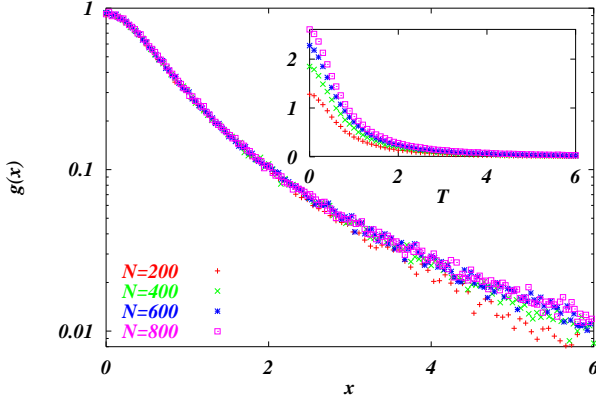


Fig. 3. Scaling function $g(x)$ in the Re-Rem. The inset shows the raw data for the mean number of crossings versus temperature for $\alpha = 0.5$.

for any α and N . Consider first the case $\alpha = 0.5$ which is the appropriate value in the mean field picture. One has

$$\mathcal{N}_N^{\alpha=0.5}(T, T + \delta T) = \sqrt{N} \delta T g(T) \quad (20)$$

Focusing on the interval $T_c/3$ to $2T_c/3$, we find about $6\sqrt{N/1000}$ crossings, that is 6 crossings for $N = 1000$.

One can also consider other values for the exponent α . In the framework of the EA model in $d = 3$, the fractal dimension of the surface of system-size domains has been measured [24, 25], leading to $\alpha = d_s/2d \approx 0.46$. For this value of the exponent the mean number of crossings in the $T_c/3$ to $2T_c/3$ interval is now reduced to about 3 when $N = 1000$.

The main conclusion of this section is that the number of crossings in a temperature interval grows as a power of N if $0 < \alpha \leq 0.5$ but with a small *prefactor*. Thus, if we simply map our Re-Rem results to estimate the strength of chaos that should arise in Monte Carlo simulations, we find that there will be very little sign of chaos until N is at least a few hundred. However, the mapping from the Re-Rem most certainly over-estimates significantly the number of crossings in microscopic models (cf. the next section and the final discussion).

5 Droplet extension of the Re-Rem

As given so far, our Re-Rem has excitation energies of $O(1)$. However, it is possible to modify the model in order to mimic the *droplet/scaling* [13, 20] picture of spin glasses. There low-lying excitation energies are $O(N^{\theta/d})$, that is $O(L^\theta)$ where θ is the stiffness exponent which is at the heart of the droplet and scaling pictures of spin glasses.

5.1 REM revisited: The Scaling-REM

To construct the Scaling-REM (S-REM), we note that it is not appropriate to identify single spin configurations with states, a valley containing a large number of similar

configurations. Thus we take a number of states that is much smaller than 2^N ; as a consequence, the variance of their energy will no longer be $O(N)$. Our method is thus to rescale the energies by a factor $N^{\theta/(2d)}$ while the number of states is reduced from 2^N to 2^{N^β} (with $\beta < 1$). This gives

$$2\sigma_E^2 = N^{1+\frac{\theta}{d}} \quad (21)$$

$$S_C(E) = N^\beta \ln 2 - \frac{E^2}{2\sigma_E^2} \quad (22)$$

Then $T_c = \sigma_E / \sqrt{2N^\beta \ln 2}$ and $E_0 = -\sigma_E \sqrt{2N^\beta \ln 2}$. We want an extensive ground state energy at $T = 0$; thus

$$E_0 = -\sqrt{N^\beta \ln 2} \sqrt{N^{1+\theta/d}} \quad (23)$$

imposes $\beta = 1 - \frac{\theta}{d}$. It follows that the critical temperature is now given by $T_c = N^{\theta/d} / (2\sqrt{\ln 2})$, and so $T_c > 0$ only if $\theta \geq 0$. Note that for $\theta > 0$, $T_c \rightarrow \infty$ as in the Directed Polymer in a Random Medium (DPRM) in 1+1 dimension, in contrast to what happens in realistic spin glasses. Actually, this S-REM is very close to the DPRM. Consider for instance the exponents giving (i) the finite size corrections to the ground state energy, (ii) the sample to sample fluctuations and (iii) the energy of the first excited state; they are the same (i.e., θ/d) in the two models, whereas two distinct exponents arise in the droplet model [26]. Nevertheless, this S-REM provides an interesting picture of the low temperature phase that is quite compatible with the scaling/droplet picture there, even if it misses $T_c < \infty$.

5.2 Re-Rem revisited

We can perform the analogous scaling extension for the Re-Rem and obtain a Scaling-Re-Rem where low-lying excitation energies scale as $N^{\theta/d}$. All the computations are straight-forward. One finds that the critical temperature of the S-Re-Rem is given by

$$T_c = \frac{\sqrt{N^{1+\theta/d} + T^2 N^{2\alpha}}}{2\sqrt{N^{1-\theta/d} \ln 2}} = \frac{N^{\theta/d} \sqrt{1 + T^2 N^{2\alpha-\theta/d-1}}}{2\sqrt{\ln 2}} \quad (24)$$

and that $F_0 \propto -N\sqrt{1 + T^2 N^{2\alpha-1-\theta/d}}$. Now letting $\alpha' = \alpha - \theta/(2d)$, we have

$$T_c = \frac{N^{\theta/d} \sqrt{1 + T^2 N^{2\alpha'-1}}}{2\sqrt{\ln 2}} \quad (25)$$

$$F_0 \propto -N\sqrt{1 + T^2 N^{2\alpha'-1}} \quad (26)$$

From this, we see that the thermodynamics is the same as that of the Re-Rem but where α has been replaced by $\alpha - \theta/(2d)$. We can also apply this correspondence to the

formulae for the level crossing properties¹, again again that there is temperature chaos. More precisely, if we start from the scaling form 16 then using α' instead of α , equation 26 implies as before that $\beta_2 = 0.5$, but $\beta_1 \neq 0$ since the width of the tube grows as $N^{\theta/d}$. However, the number of levels being 2^{N^β} , the total number of crossing goes as $\sqrt{N^\beta}$ and the general scaling for $\theta \neq 0$ is

$$\mathcal{N}_N(T, T + \delta T) = N^{\alpha - \theta/d} \delta T g\left(\frac{T}{N^{0.5 - \alpha + \theta/2d}}\right) \quad (27)$$

5.3 Criterion for temperature chaos

Even if the S-Re-Rem model is a bit ad-hoc, it may correctly describe some glassy systems at low temperature. The general criterion for temperature chaos depends only on the value of parameters α and θ/d . If $\alpha - \theta/d < 0$, there is no chaos at all, all crossings being pushed to $T = \infty$. If $\alpha - \theta/d = 0$, the density of crossings is finite; this is what we call *weak temperature chaos*. If $0 < \alpha - \theta/d$ while $\alpha - \theta/(2d) \leq 0.5$, there are an infinite number of crossings in each temperature interval, that is *strong temperature chaos*. Finally, if $\alpha - \theta/(2d) > 0.5$, there is *no finite temperature chaos* because all crossings take place at $T = 0$. Note that if one accepts $\alpha = d_s/2d$, we recover the original Bray and Moore argument. However, within our model we can estimate the number of crossings, and comparing to the discussion of section 4, the case $\theta > 0$ leads to even fewer crossings than when $\theta = 0$.

6 Temperature chaos in the naïve mean field framework

Ideally, one would like to confront the Re-Rem predictions with the chaos properties arising in a realistic model. This requires defining finite volume states or valleys and following them as a function of temperature. A natural approach is to use the TAP [19] equations where each state is parametrized by its magnetizations $m_i = \langle S_i \rangle$. However, these equations have 2 serious drawbacks: (i) on the 3-dimensional lattice, the TAP equations fail to give non-paramagnetic solutions [27]; (ii) even for the SK model [28], having $N < \infty$ (which is unavoidable numerically) leads to unsurmountable convergence problems [29]. The source of these difficulties seems to be the strength of the retro-action term. An ad-hoc solution consists in either reducing or neglecting this term. Following previous authors [27, 30], we choose the second option which corresponds to the naïve mean field equations (NMFE) [31].

6.1 Naïve Mean Field Equations

The NMFE are

$$m_i = \tanh\left(\beta \sum_j J_{ij} m_j\right) \quad (28)$$

¹ Note that the width of the tube now grows as $N^{\theta/d}$.

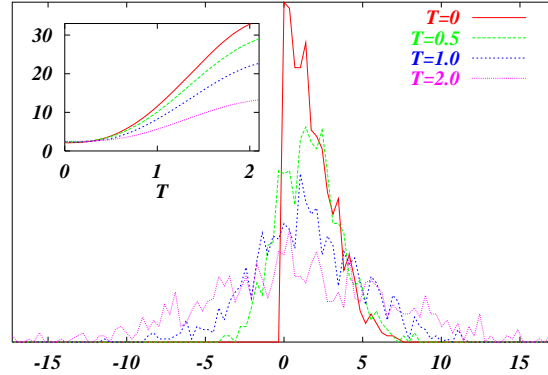


Fig. 4. $P(\delta F)$ at different temperatures for $0 \leq |q| \leq 0.05$ excitations in L=12 EA model. Inset: the variance of δF for $L = 8, 10, 11$ and 12 (from bottom to top).

The solutions to these equations define the naïve mean field (NMF) states; they correspond to the stationary points of the NMF free-energy functional

$$F(\{m_i\}) = E(\{m_i\}) - TS(\{m_i\}) \quad (29)$$

where the energy and the entropy functionals are given by

$$E = - \sum_{\langle ij \rangle} J_{ij} m_i m_j \quad (30)$$

$$S = - \sum_i \frac{(1 + m_i) \ln(1 + m_i) + (1 - m_i) \ln(1 - m_i)}{2} \quad (31)$$

F has both local minima and saddles; we follow the TAP approach and construct in our numerics only local minima.

Our procedure is as follows. For each disorder instance, we will produce two NMF states \mathcal{L}_1 and \mathcal{L}_2 and will work out their dependence on temperature. We start by building their $T = 0$ intercept: \mathcal{L}_1 is in fact the ground state, while \mathcal{L}_2 is a large-scale low-energy excitation. (To obtain the ground state, we use a state-of-art algorithm [32]. In virtue of the method used to generate excitations [24], the excitation energies are $O(1)$ and do *not* grow when increasing N .) We then numerically determine how the \mathcal{L}_i evolve as we increase the temperature from 0 to T_c . In practice, we increase the temperature T in sufficiently small steps ($\Delta T = 0.05$) and perform steepest descent on the free-energy functional, using as starting point \mathcal{L}_i at the previous temperature. With this procedure, referred to as *heating* of the ground state in [30], we consider two NMF states that evolve with increasing temperature.

6.2 Numerical results for the 3 - d EA model

First, let us give some qualitative properties of this NMF system. We find a non-zero Edwards-Anderson order parameter $q_{EA} = \sum_i m_i^2 / N$ for any instance and any state

when $T < T_c$ ($T_c \approx 5$ in the 3-d NMF EA model, and $T_c \approx 2$ in the NMF SK model), and q_{EA} is self-averaging. If we follow a given state, the two temperature spin overlap $q_{0T} = \sum_i m_i^{(T=0)} m_i^{(T)}/N$ decreases and reaches zero when $T = T_c$. Furthermore, the equal temperature mutual overlap between \mathcal{L}_1 and \mathcal{L}_2 , $q_{TT}^{\alpha\beta} = \sum_i m_i^\alpha(T) m_i^\beta(T)/N$, also decreases smoothly when going from $T = 0$ to T_c , suggesting that evolving those states according to the NMF equations mainly just reduces the size of the $m_i = \langle S_i \rangle$. Do we get level crossings as would be expected if there was temperature chaos? We are particularly interested in the behavior of state to state free-energy fluctuations at very low temperatures as this quantity is at the heart of our Re-Rem picture.

For this model, we have used on average 1000 ground states and excitations for sizes $L = 8, 10, 11$ and 12. We focus in all that follows on the instances where our excitations have an overlap with the ground state satisfying $0 \leq |q| \leq 0.05$. However the data for other overlap intervals have a qualitatively similar behavior.

According to zero-temperature chaos, when going from $T = 0$ to $T > 0$, the valley \mathcal{L}_1 should be above the valley \mathcal{L}_2 with a strictly positive probability when N grows. We find this to be the case, and have found that the probability to find such an inversion increases with temperature. To understand this more quantitatively, define δF to be the free-energy difference $F(\mathcal{L}_2) - F(\mathcal{L}_1)$. Figure 4 shows the distribution $P(\delta F)$ at different temperatures for $L = 12$. The variance of this distribution increases with temperature. The curves for different L and different window overlaps look similar, so once $T > 0$, there is a positive probability that $\delta F < 0$, corresponding to a level crossing. Since there are an infinite number of such excitations in the thermodynamics limit, and since they plausibly all behave the same way, these crossings suggest that there is indeed temperature chaos.

To make contact with our Re-Rem picture, one should extract α from the L dependence of the variance of δF . If $\alpha > 0$, the variance of δF will diverge at large L as $L^{2\alpha d}$. In the inset of figure 4 we plot the variance of δF at different temperatures. At any given temperature, we can fit its L dependence; not surprisingly, just as was previously found at $T = 0$ [24, 25], the data can be fit with $\alpha = 0.5$ (the mean field case $d = d_s$) while the best fit gives $\alpha \approx 0.46$ ($d_s \approx 2.76$). What is important is that α is certainly not 0. This suggests that this system have strong chaos.

6.3 Numerical results for the SK model

Recently, the naïve mean field framework was used by Mulet *et al.* [30] to study temperature chaos in the SK model. Although they concluded that there is no chaos, we feel it is necessary to reconsider that conclusion in view of the Re-Rem analysis.

Compared to the EA model, the SK is numerically difficult because of its long range interactions. More numerical effort is needed to find ground states or excitations and also for doing the steepest descent on the NMF free-energy functional. We were thus limited to “small” values

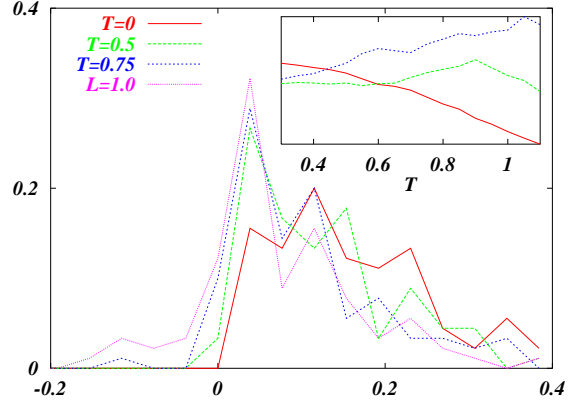


Fig. 5. $P(\delta F)$ at different temperatures for $0 \leq |q| \leq 0.05$ excitations in the SK model ($N = 192$). Inset: the variance of δF for $L = 64, 128$ and 192 as a function of T (bottom to top).

of N : we used $N = 64, 128$ and 192 , performing statistics using 50 ground states and excitations for each value of N .

Our conclusions are qualitatively similar to those we obtained for the 3-d EA model (see figure 5). We find that there is a strictly positive probability that \mathcal{L}_1 and \mathcal{L}_2 cross; fits of the free-energy fluctuations give a value for α fully compatible with 0.5. These results are those that are expected in the Re-Rem picture; it is thus appropriate to conclude that there *should be* temperature chaos. However, note that the variance of δF grows only slowly with N so very few crossings are expected until much larger values of N are reached.

7 Discussion

This work has two main points. First, we have developed a solvable model of spin glasses inspired from the REM that allows a precise study of temperature chaos. This model has strong temperature chaos unless its exponent α is artificially set to zero. However; this chaos is absent until the system size N reaches about several hundred. Second, we have argued that this Re-Rem model should be relevant for real spin glasses by considering the particular case of naïve mean field equations. The numerical study of that system turned out to be in complete agreement with the expectations of the Re-Rem picture, giving strong evidence that temperature chaos does occur in spin glass models such as the 3-d Edwards-Anderson and the SK models.

The question of temperature chaos has lingered on for many years because of lack of numerical evidence. One may considering the absence of chaos signals in past and present MC simulations by the fact that in the Re-Rem, N must be quite large for chaos to appear. Indeed, we saw that in the Re-Rem chaos becomes clear for $N \simeq 1000$ but it is clearly inappropriate to consider that one has 2^N states in a physical system of N spins. Having far fewer states will lead to fewer crossings, and so it may be that

no chaos will be seen from MC simulation in the near future. However, we believe that our naïve mean field study suggests on the contrary that chaos in realistic systems is within grasp of current Monte Carlo techniques. One way to do this is to consider for instance the $3 - d$ EA model and to extract at each temperature the states or “valleys” by clustering the equilibrium configurations. Then following these states in temperature will allow one to compare directly with the Re-Rem picture.

In the future, it would be interesting to extend the Re-Rem to more complex systems such as the Generalized Random-Energy-Model. In such a G-Re-Rem model, one would be able to understand the effects of 2-step, 3-step and continuous RSB. Another interesting possibility is to study the Re-Rem with more realistic behavior than a pure linear dependence in T , the free-energies of levels being a more complicated function of T .

Acknowledgments

We wish to thank M. Mézard, G. Parisi and M. Sasaki for stimulating discussions. F.K. acknowledges a fellowship from the MENRT. The LPTMS laboratory is an Unité de Recherche de l’Université Paris XI associée au CNRS.

Appendix

Here we explain in detail our algorithm. We want to construct efficiently the series of crossing points for a realization of the Re-Rem having 2^N states or levels, level i having energy E_i and entropy S_i . It is convenient to assume that these states have been ordered in increasing value of their energies. We will start with the ground state: this level $l(0) = 0$ has energy-entropy $(E_{l(0)}, S_{l(0)})$. Then we will continue by finding the next level $l(1)$ that has a lower entropy than that of $l(0)$, i.e., $S_{l(1)} < S_{l(0)}$. This construction is extended by recurrence: given the level number $l(n)$ and values $(E_{l(n)}, S_{l(n)})$, we will generate with the correct probability distribution of the next level $l(n+1)$ that has $S_{l(n+1)} < S_{l(n)}$ as well as the quantities $(E_{l(n+1)}, S_{l(n+1)})$. The key point is that all these quantities can be generated recursively without “looking” at all 2^N states. Once this list of $(l(n), E_{l(n)}, S_{l(n)})$ values is constructed (this takes $O(N)$ operations), we can then reconstruct the lowest state at any temperature, and thus the statistics of the crossings.

To begin our algorithm, we set $n = 0$, $l(0) = 0$ and choose $S_{l(0)}$ according to its Gaussian distribution. Then we must generate $E_{l(0)}$ (note that $E_{l(0)}$ and $S_{l(0)}$ are uncorrelated random variables). The probability density of $E_{l(0)}$ is

$$P(E_{l(0)}) = 2^N \rho_N(E_{l(0)}) [1 - Q(E_{l(0)})]^{(2^N - 1)} \quad (32)$$

where $\rho_N(E)$ is the probability density of energies in the Re-Rem model (a Gaussian) and Q is defined by

$$Q(E) = \int_{-\infty}^E \rho_N(x) dx \quad (33)$$

To generate $E_{l(0)}$ with its distribution, we use the accept/reject method. Finally we set $E_{old} = E_{l(0)}$ and $S_{old} = S_{l(0)}$.

Now we enter the recursion. Given the values $l(n)$, E_{old} and S_{old} , we first determine the next level $l(n+1)$ that has an entropy below S_{old} . Let Δl be defined by $l(n+1) = l(n) + \Delta l$; Δl is exactly the number of times one has to generate a random entropy S_{new} according to the Re-Rem entropy distribution until we find a value satisfying $S_{new} < S_{old}$. Define p to be the probability to get a slope smaller than S_{old} with *one* trial; then

$$p = \int_{-\infty}^{S_{old}} \rho_N(S) dS \quad (34)$$

Clearly, Δl (the number of attempts made before reaching an entropy value lower than S_{old}) is a random variable; its probability distribution is

$$P(\Delta l) = (1 - p)^{\Delta l - 1} p \quad (35)$$

We thus generate Δl according to this distribution. This gives us the new level to consider, $l(n+1) = l(n) + \Delta l$. If $l(n+1) \geq 2^N$, we stop as such a level does not exist. Otherwise, $l(n+1)$ is a legitimate level, and we proceed by determining $(E_{l(n+1)}, S_{l(n+1)})$.

The *entropy* of level $l(n+1)$ is easy to generate because its distribution is that of any S_i subject to the condition that $S_{new} < S_{old}$. The only difficulty is for generating $E_{l(n+1)}$. To do that, start with $P(E_{old}, E_{new}) = P(E_{old})P(E_{new}|E_{old})$ where the quantities $l(n)$ and $l(n+1)$ are considered as known. From this relation, we derive

$$\begin{aligned} P(E_{new}|E_{old}) &= \binom{l(n+1) - l(n) - 1}{M - (l(n) + 1)} \\ &\times Q(E_{old}, E_{new})^{\Delta l - 1} (M - l(n + 1)) \rho_N(E_{l(n+1)}) \\ &\times \frac{(1 - Q(E_{l(n+1)}))^{M - (l(n+1) + 1)}}{(1 - Q(E_{l(n)}))^{M - (l(n) + 1)}} \quad (36) \end{aligned}$$

when $M = 2^N$ and $Q(a, b) = Q(b) - Q(a)$. We sample this distribution by the accept-reject method again.

Equation 35 has a simple interpretation; we have built a set of “volumes” in the space of E_i s. The relative space we can explore now has weight $[1 - Q(E_{l(n)})]^{M - (l(n) + 1)}$. In this space, we first generate $\Delta l - 1$ energies in the interval $[E_{l(n)}, E_{l(n-1)}]$ and this gives the first part. Then we assign the level whose energy is $E_{l(n+1)}$. There are $M - l(n + 1)$ ways to choose the level among the remaining ones. Finally, the last $(M - (l(n + 1) + 1))$ energies have to be assigned and then we must normalize the distribution. Given this E_{new} , we set $E_{l(n+1)}$ to E_{new} and we are finished. To continue the recursion, we set E_{old} to E_{new} , S_{old} to S_{new} and n to $n + 1$.

To summarize the whole procedure, using these probability distributions, we can directly create an instance of a list of crossings by producing the $O(N)$ $E_{l(n)}$ and $S_{l(n)}$ that will cross and then study these crossings (this is a simple problem). From a numerical point of view however, these distributions are not so easy to compute, and one has to take care of machine rounding errors; that source of error limited us to $N < 1000$.

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